

ABSTRACT

The invention relates to a method for creating a database enabling, in particular, the selection of at least one reaction-capable catalyst, comprising the following steps: a) preparing a number of different reaction media containing the same reactivity probe and each having at least one catalyst; b) analyzing, by means of an analytic method, each reaction medium after reaction, and; c) assigning, in the database, an analysis result according to step b) to the reactivity probe, this result characterizing different reaction products obtained from said reactivity probe. The database is a relational database containing: a first entity in which items of information relative to the reaction patterns listed in the data base are recorded; a second entity containing items of information relative to the state of bindings of at least one reaction pattern listed in the first entity; a third entity in which items of information associated with different reaction media are stored, and; at least one fourth entity in which items of information are stored that are linked to the analysis results of the reaction media at the end of a reaction.